Infrared Spectroscopy Applied in the Authentication of Genuine Edible Sesame Oil

Abstract:

Country C is a major consumer of sesame oil, yet in recent years, there has been a recurring issue of adulteration in the market, with instances of either adulterated sesame oil or the direct substitution of low-quality, cheaper vegetable oils for sesame oil. To safeguard the interests of consumers and legitimate businesses, it is imperative to research rapid and accurate methods for authenticating and detecting adulteration in sesame oil.

Currently, gas chromatography is a common method for the authentication and adulteration analysis of oils. However, the analysis steps in gas chromatography are relatively complex, time-consuming, costly, and might not meet the requirements for rapid detection. Infrared spectroscopy technology offers non-destructive, rapid, and convenient characteristics. In recent years, with the continuous development of hardware (interferometers and various infrared accessories) and software technologies (Fourier transform and chemometrics), the combination of FTIR and chemometrics has become an effective means of analyzing the quality of edible oils.

This project attempts to practically utilize the characteristic features of mid-infrared spectroscopy and the powerful discriminatory ability of chemometrics for authenticating edible sesame oil.

In this study, eleven samples from ten different brands (A, B, C, D, E, F, G, H, I, J) and ten adulterated sesame oil samples were investigated. Spectral scans of the samples were conducted using mid-infrared spectroscopy, and chemometric methods were employed for pattern recognition of the oil samples. The results indicate that the discriminant model established using chemometric software can accurately identify branded sesame oil at a rate of 94.03% and adulterated sesame oil at a high rate of 97.25%. The practical effect of this approach proves to be highly promising.

Keywords:

Mid-infrared spectroscopy, sesame oil, authenticity determination, chemometrics

1. Experimental Conditions

1.1 Materials and Methods

Branded sesame oil was procured from legitimate sources, including ten brands (A, B, C, D, E, F, G, H, I, J), totaling eleven samples. Representative adulterated samples were obtained from relevant

national quality inspection departments. All samples were stored at room temperature between 20°C to 25°C.

1.2 Instrumentation and Accessories

FTIR-7600S Fourier Transform Infrared Spectrometer;

Liquid Testing Attachment: Single Reflection ATR Accessory (ZnSe crystal, 45° incident angle);

1.3 Test Conditions

Resolution: 4 cm-1

Number of Scans: 64 times

2. Spectrum Analysis

2.1 Overlay of Test Spectra

2.2 Similarity Analysis

Conducting similarity analysis on two types of samples shows, as depicted in the figure above, that with the exception of very few non-representative data points, there is no significant overall difference between the branded sesame oil and the adulterated sesame oil samples. Therefore, employing different algorithms in the similarity function directly does not achieve the goal of distinguishing between branded sesame oil and adulterated sesame oil.

2.3 Multivariate Statistical Analysis

Based on the similarity analysis results in 2.2, where there isn't a significant difference between branded sesame oil and adulterated sesame oil, an attempt was made to process the data using multivariate statistical analysis to achieve the intended goal.

Discriminant Partial Least Squares (PLS-DA) was employed to analyze the two types of sesame oil samples, as depicted in the figure above. While there is some overlap in a small portion of the data, overall, branded sesame oil and adulterated sesame oil can be separated into two categories.

2.4 Classification Pattern Recognition

(1) Identification of Branded Sesame Oil

Using the test set data of branded sesame oil and adulterated sesame oil with the Partial Least Squares algorithm for pattern recognition, the results are as depicted in the figure. Among the 134 data points in the test set, only 8 were inaccurately identified, resulting in a recognition rate of 94.03%, meeting the expected performance.

(2) Identification of Adulterated Sesame Oil

Utilizing the Partial Least Squares algorithm for pattern recognition using the training set data of branded sesame oil and adulterated sesame oil, the results are depicted in the figure. Among the 109 data points in the test set, only 3 were inaccurately identified, resulting in a high recognition rate of 97.25%, meeting the expected performance.

3. Conclusion:

This study focused on 11 samples from 10 brands, alongside 10 adulterated sesame oil samples. Mid-infrared spectroscopy was employed for spectral scanning of the samples, combined with chemometrics for pattern recognition of sesame oil samples. The results demonstrate that the discriminant model established using chemometrics software can accurately differentiate between branded sesame oil and adulterated sesame oil. The recognition rate for branded sesame oil reached 94.03%, while the recognition rate for adulterated sesame oil was as high as 97.25%, indicating highly favorable determination outcomes.